An Effective Theory for Midgap States in Doped Spin Ladder and Spin Peierls Systems: Liouville Quantum Mechanics

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Abstract

In gapped spin ladder and spin-Peierls systems the introduction of disorder, for example by doping, leads to the appearance of low energy midgap states. The fact that these strongly correlated systems can be mapped onto one dimensional noninteracting fermions provides a rare opportunity to explore systems which have both strong interactions and disorder. In this paper we will show that the statistics of the zero energy midgap wave functions $\psi_0(x)$ in these models can be effectively described by Liouville Quantum Mechanics. This enables us to calculate averages over disorder of the products $\psi_0^2(x_1)\psi_0^2(x_2)...\psi_0^2(x_N)$ (the explicit calculation is performed for $N = 2, 3$). We find that whilst these midgap states are typically weakly correlated, their disorder averaged correlations are power law. This discrepancy arises because the correlations are not self-averaging and averages of the wave functions are dominated by anomalously strongly correlated configurations; a fact which is not always appreciated in the literature.

1 Introduction

One dimensional quantum spin systems have long fascinated both theorists and experimentalists; more recently there has been particular interest in the behaviour of such systems in the presence of disorder (see eg. [1] and references therein). There are several reasons for this, but one significant motivation is the comparatively recent experimental realisation of doped quasi-one-dimensional spin-Peierls and spin ladder systems [2]. One of the most important general results in these materials is the appearance upon doping of magnetic states at energies well below the spin gap- which dramatically changes their magnetic properties (see eg. [3] and references therein).

As well as the new results emerging from experiment, theoretical work has revealed many unusual features in a range of different one dimensional disordered spin models. Prominent among these results is the occurrence of Griffiths phases; here the low energy response is dominated by anomalously strongly correlated regions of the system. The property related to that is a sharp distinction between *typical* and *disorder averaged* correlations; the latter are much stronger and typically power law at criticality [1]. The fact that the correlation functions are not "self-averaging" means that rare strongly correlated configurations dominate the disorder averaged quantities. Thus the disorder averaged correlations can be much stronger than one would naively guess based on the implicit assumption that "averaged" and "typical" are the same thing. This is important because it is these averaged correlations which will be relevant in experiments.

Our approach to these one dimensional spin systems is to exploit the various mappings to fermionic theories. This provides an alternative way of thinking about the problem which can be related to the extensive body of literature on disordered fermion systems. The spin sector of both the two chain spin ladder [4] and the spin-Peierls system [5] can be represented in terms of massive noninteracting fermions. When these systems are lightly doped their conductivity shows variable range hopping behaviour, which means that the charge carriers are strongly localised and no band forms. Thus to investigate magnetic properties it is reasonable to continue to work with a pure spin model without fluctuations in the charge sector.

We will argue that doping with nonmagnetic impurities can be represented by a type of randomness in the mass of the fermions of the effective theories [4],[5]. Specifically the mass has fixed magnitude m_0 (the value of

the undoped spin gap) except that it flips between $+m_0$ and $-m_0$ at the locations of impurities such that $\langle m \rangle = 0$. This nontrivial background admits localised low energy states well below the gap in addition to the massive bulk modes.

It is useful to comment briefly on some insights from the theory of electrons in disordered metals, in order to better understand the connection with spin theories. One of the reasons that this problem is so complex is the existence of many different length scales. A great deal is known about the behaviour of metallic-type extended states which explore the whole sample, i.e. the limit of small wavefunction amplitudes $t = |\psi(x)|^2$; this depends only upon the global symmetry of the ensemble and can be derived from random matrix theory (see eg. [6] and references therein).

However, at length scales much less than the localisation length L_c but much larger than the mean free path l, strongly localised states with anomalously high local amplitude are important (in the conventional localisation this situation emerges when disorder comes from scattering on magnetic impurities). These states look far from metallic in the region $l \ll L < L_c$ and their correlations are sensitive to local variations in the potential; this is essentially the origin of the distinction between *typical* and *disorder averaged* correlation functions in this regime [7]. This is in sharp contrast to the behaviour of metallic states which are equally affected by the random potential at all points in the sample, and not surprisingly the wavefunction statistics are no longer simple. Here we can see a relation with the behaviour of 1d disordered spin systems; it is this kind of state which corresponds to localised low energy spin degrees of freedom.

Recent work on this problem using a variety of approaches has shown that the wavefunction statistics in this regime can be described by Liouville field theory [8] and that, for example in the two dimensional case relevant to the quantum Hall effect, one observes such interesting phenomena as multifractality [7],[8].

It was pointed out in [9] that in a system of one dimensional fermions with random mass m and $\langle m \rangle = 0$, the Lyapunov exponent $\gamma(E) \sim 1/(-\ln E)$ tends to zero as $E \to 0$ and so for low energies we are always at length scales much less than the localisation length $L_c \sim 1/\gamma$. Thus it is not at all surprising that in one dimensional systems of length $L > l$ we see a departure from the universal features predicted by random matrix theory [6].

In this paper we will study one dimensional Dirac fermions with a random

mass. We show that the correlation functions of the so-called prelocalised zero energy states can be calculated using as an effective theory Liouville quantum mechanics. This analysis is rather general and does not depend upon the specific form of the disorder. In section (3) we will then describe the application of these results to spin systems; here the low energy states represent the midgap magnetic states mentioned above. The advantage of this approach to the midgap states is that it enables us to get a clear picture of their behaviour and specifically their correlations, information which is hard to obtain using more traditional methods.

2 Effective Theory

Suppose we have a system of 1+1 dimensional non-interacting Dirac fermions with a random position dependent mass. The Hamiltonian can be written;

$$\mathcal{H} = \int dx \psi^\dagger \left(-i\sigma^2 \frac{\partial}{\partial x} + \sigma^1 m(x) \right) \psi \tag{1}$$

$$\psi(x) = \begin{pmatrix} u(x) \\ v(x) \end{pmatrix} \tag{2}$$

where σ^1 and σ^2 are the standard definitions of the Pauli matrices. This leads to the equations of motion, in component form;

$$\begin{aligned} \left(\frac{d}{dx} + m(x) \right) u(x) &= Ev(x) \\ \left(-\frac{d}{dx} + m(x) \right) v(x) &= Eu(x) \end{aligned} \tag{3}$$

Even if $m(x)$ is finite and nonzero almost everywhere, if it passes through zero at some points there will be normaliseable bound states with energy close to zero- midgap states. This can be seen from replica, supersymmetry and numerical calculations where a peak appears in the density of states at $E = 0$ (see eg. [9] and references therein). However, within these approaches it is notoriously difficult to calculate the correlation functions.

It is remarkable that one of the low energy solutions of eqs.(3) can be explicitly written down; it is the zero energy eigenmode;

$$\psi_0(x) = \frac{1}{\mathcal{N}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \exp\left(-V(x)\right) \tag{4}$$

$$V(x) = \int_0^x m(y)dy \tag{5}$$

$$\mathcal{N}^2 = \int_0^L dx \exp\left(-2V(x)\right) \tag{6}$$

Here it is our purpose to calculate correlations of these zero energy eigenstates for the case where $\langle m \rangle$, the average mass is zero.

In disordered systems, we are usually interested in *disorder averaged* correlations. Here as always the difficulty is to correctly account for the normalisation factor (denominator) in the average. Following Kogan, Mudry and Tsvelik [8] we introduce a dummy variable μ which allows us to transfer all the $V(x)$ dependence from the denominator into the numerator; a disorder average can then be performed.

In the continuum limit, it is apparent that the quantity $V(x)$ (5) will behave like the position variable in a random walk [10], where x is the "time" coordinate. Therefore, going to a path integral formulation we find in the continuum limit the following Gaussian probability distribution for V (for more details see [10]);

$$P(\{V\})DV = \exp\left[-\frac{1}{2g}\int dx(\partial_x V)^2\right] DV \tag{7}$$

where g parametrises the strength of the disorder. This will be valid for sufficiently long distances in the correlation functions; different realisations of disorder may give rise to different behaviours at small separations. In the case of "telegraph disorder" where m randomly assumes either $\pm m_0$, $g = \frac{\hbar^2 m_0^2 a_0}{v^2}$ where a_0 is the lattice spacing and v is the velocity in the Dirac equation (2) (often taken as 1 for simplicity). For more general forms of disorder, g will roughly speaking be larger for broader distributions of m. Note that g is independent of impurity density- this will however affect the length scales above which the distribution (7) is valid.

Then the disorder averaged correlator ($\langle X \rangle$ denotes the disorder average of the quantity X) ;

$$\langle |\psi_0(x_1)|^2 ... |\psi_0(x_N)|^2 \rangle = \int DV P(\{V\}) |\psi_0(x_1)|^2 ..... |\psi_0(x_N)|^2 \tag{8}$$

can be expressed as

$$\langle |\psi_0(x_1)|^2 ... |\psi_0(x_N)|^2 \rangle = \int_0^\infty \frac{d\mu \exp[-\alpha\mu]\mu^{N-1}}{(N-1)!} \times \int DV \prod_{i=1}^{N} \mathrm{e}^{-2V(x_i)} \mathrm{e}^{-S_\mu}$$

(9)

where α is introduced to regularise the μ integral and

$$S_\mu = \int dx \left[\frac{1}{2g} (\partial_x V)^2 + \mu \exp(-2V) \right] \tag{10}$$

is the action of Liouville quantum mechanics [13] where x is the "time" coordinate.

We can now go to the canonical Hamiltonian form;

$$\mathcal{H} = -\frac{g}{2} \frac{d^2}{dV^2} + \mu \exp(-2V) \tag{11}$$

and find the eigenstates of the effective theory, which allows us to calculate the correlation functions. The detailed calculation of the one,two and three point correlators is described in the Appendix. In fact all of the correlators are proportional to a constant factor which depends upon an integral over the dummy variable μ (which must be suitably regularised) and an unspecified normalisation factor A. Since the same factor appears in front of all the correlators, we may fix its value by insisting that the wavefunctions are correctly normalised:

$$\int dx \langle |\psi_0(x)|^2 \rangle = 1 \tag{12}$$

hence

$$\langle |\psi_0(0)|^2 \rangle = \frac{1}{L} \tag{13}$$

where L is the size of the system. Comparing this with the result of A2, Eq. (33) we find for the two and three point correlators the following correctly normalised power law behaviour:

$$\langle |\psi_0(x_2)|^2 |\psi_0(x_2)|^2 \rangle = \left(\frac{1}{L} \frac{g}{16\sqrt{2\pi}} \right) \left(\frac{1}{g x_{21}} \right)^{\frac{3}{2}} \tag{14}$$

$$\langle |\psi_0(x_3)|^2 |\psi_0(x_2)|^2 |\psi_0(x_1)|^2 \rangle = \left(\frac{1}{L} \frac{g^2}{1024} \right) \left(\frac{1}{g x_{32}} \right)^{\frac{3}{2}} \left(\frac{1}{g x_{21}} \right)^{\frac{3}{2}} \tag{15}$$

where we have chosen without loss of generality $x_3 > x_2 > x_1$ and $x_{ij} = x_i - x_j$, and the derivation assumed that $|gx_{ij}| \gg 1$, $i \neq j$. This is a very clear example of the important difference between *typical* and *disorder averaged* correlations. From the expression (4) we would expect the typical correlations to decay exponentially. What happens is that atypical strongly correlated configurations dominate the average and give much stronger power law correlations in the disorder averaged quantities.

3 Application to Spin Systems

We discussed in the introduction some of the characteristic features of one dimensional disordered spin systems including the occurrence of Griffiths phases, and the related distinction between typical and averaged correlation functions. As we have seen a similar picture holds for the correlations of low energy fermion modes in one dimension; and this is not a coincidence but an expression of the deep relationship between certain one dimensional spin systems and systems of fermions.

Since the analysis above is equally valid for Majorana (real) fermions, one can first of all make the direct observation that this model with random mass is equivalent to the quantum Ising model with random bonds. This has been studied by many authors (including eg [1], [14]). In particular Shankar and Murthy [14] found that the typical correlation functions of fermion bilinears decayed exponentially as the square root of distance as one would expect; our result shows in addition that at criticality the disorder averaged correlation functions of zero energy modes are power law.

Let us now consider the doped spin-Peierls and spin ladder systems. Fabrizio and Mélin [5] have suggested that one can gain insight into the spin-Peierls system by considering the XY version- this maps to to a system of noninteracting massive Dirac fermions whose mass is proportional to the dimerisation. They argue that the introduction of impurities can be modelled simply by the presence of domain walls between vacua with dimerisation of opposite sign. This leads to a model of fermions with a mass which flips between $+m_0$ and $-m_0$ at impurities (by symmetry $\langle m \rangle = 0$); one finds low energy midgap states localised in regions with impurities, of which the zero energy eigenstate considered in this paper is one example.

In the language of spins these midgap states correspond to the effective

spins which appear at breaks or discontinuities in gapped spin chains [3], since for this model the z component of the magnetisation S^z is proportional to the fermion density.

These impurity spins are often treated in the literature as though they are essentially uncorrelated, based on the argument that they are *typically* weakly coupled for low impurity density. We emphasise again that whilst this is true, our work shows that their disorder averaged correlations are power law; and these are the relevant quantities in experiment. It is for this reason, for example that they do not give a simple Curie contribution to the susceptibility; Fabrizio and Mélin [5] showed that $\chi(T) \sim 1/(T \ln^2 T)$ a result which differs significantly at low temperatures from the noninteracting $1/T$ result.

Of course in reality the problem of spin-Peierls systems is more complicated- there are very important three dimensional effects and thermal fluctuations of the lattice distortion. It is also unclear, even in an inherently one dimensional system, whether the introduction of impurities can really be represented so simply [5]. Nonetheless we would argue that we have captured a crucial feature; which is that at boundaries between the two degenerate ground states (domain walls $\equiv$ kinks in the fermion mass) we find localised magnetic low energy degrees of freedom.

Similar arguments applied to a fermionic model of the two chain spin ladder [4], where doping is introduced in the form of static kinks in the charge field, leads again to a model of fermions with mass flipping between $-m_0$ and m_0 at the location of impurities. This can be seen from the bosonisation formalism, treating nonmagnetic impurities in a way suggested by Fukuyama *et al.* [11]. At half filling in a spin ladder system, the charge modes will be frozen (gapped). Nonetheless, because the charge density is proportional to the gradient of the charge field, a nonmagnetic charged impurity (hole) can be represented as a static kink in the field. This assumes that there are sufficiently few impurities and that they are sufficiently strongly localised so that no band forms- these conditions appear to be satisfied in typical experimental systems [2].

By taking these kinks into account in the effective theory of [4], it can be seen that their effect is to introduce kinks in the mass of the fermions describing the spin sector [12].

The interpretation in terms of spins is much as for the spin-Peierls system. In the effective theory [4], the slow component of the magnetisation is

essentially proportional to the fermion density, and so these localised states can again be interpreted as low energy spin degrees of freedom.

4 Conclusions

We have shown that Liouville quantum mechanics can usefully be applied to calculate the properties of the zero energy localised states in a model of Dirac fermions with random mass. We have emphasised the relation of this model to some one dimensional disordered spin systems; one of the most important points is that at the critical point ($\langle m \rangle = 0$) we find power law correlations for the disorder averaged correlation functions, even though typical correlations decay exponentially. This shows that even if midgap states are typically weakly correlated, anomalously strongly correlated configurations can dominate in physical quantities.

Finally, it is very interesting in itself that one can derive an effective theory for midgap states with nontrivial, calculable correlation functions; although a limitation of our approach is that it only gives information about states with energy $E = 0$. It would be very interesting if the current approach could be extended to investigate states with finite energy.

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A Calculation of Correlators

A.1 Two Point Correlator

$$C_{21} = \langle |\psi_0(x_2)|^2 |\psi_0(x_1)|^2 \rangle \tag{16}$$

$$C_{21} = \int \mu d\mu \mathrm{e}^{-\alpha\mu} M_2 \tag{17}$$

$$M_2 = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} dV_1 dV_2 \langle 0|_2 \mathrm{e}^{-2V_2(x_2)}|u\rangle_2 \langle u|_1 \mathrm{e}^{-2V_1(x_1)}|0\rangle_1 \quad (18)$$

$$= \int_0^{+\infty} dE \left| \int_{-\infty}^{+\infty} dV \langle 0|\mathrm{e}^{-2V(0)}|u\rangle \right|^2 \mathrm{e}^{-Ex_{21}} \quad (19)$$

where $E = gu^2/2$, we have chosen without loss of generality $x_{21} = x_2 - x_1 > 0$ and the energy normalised eigenstates of Liouville quantum mechanics at $x = 0$ are given as follows [13];

$$|0\rangle = AK_0\left(\sqrt{\frac{2\mu}{g}}\mathrm{e}^{-V}\right) \quad (20)$$

$$|u\rangle = \left[\frac{1}{2\pi g}\sinh \pi u\right]^{\frac{1}{2}} K_{iu}\left(\sqrt{\frac{2\mu}{g}}\mathrm{e}^{-V}\right) \quad (21)$$

where A is a normalisation which we can fix later. The "time" (x) evolution of these states is denoted by subscripts on the bras and kets:

$$|u\rangle_i = \mathrm{e}^{-Ex_i}|u(V = V_i)\rangle \quad (22)$$

First let us work out the integral over V, making the substitution $x = (\sqrt{2\mu/g})\mathrm{e}^{-V}$;

$$I = \int_{-\infty}^{+\infty} dV \langle 0|\mathrm{e}^{-V}|u\rangle \quad (23)$$

$$I = \frac{Ag^{\frac{1}{2}}}{2\pi\mu}\left[\sinh \pi u\right]^{\frac{1}{2}} \int_0^{+\infty} xK_0(x)K_{iu}(x)dx \quad (24)$$

Which gives [15];

$$I = \frac{Ag^{\frac{1}{2}}}{8\pi\mu}\left[\sinh \pi u\right]^{\frac{1}{2}} \left(\frac{\frac{\pi u}{2}}{\sinh \frac{\pi u}{2}}\right)^2 \quad (25)$$

So now

$$M_2 = \frac{A^2 g^2}{8\pi\mu^2}\int_0^{+\infty} udu \sinh \pi u \left(\frac{\frac{\pi u}{2}}{\sinh \frac{\pi u}{2}}\right)^4 \exp(-\frac{gx_{21}}{2}u^2) \quad (26)$$

For long distances $gx_{21} \gg 1$ the Gaussian factor in the integrand is very rapidly decaying, so the other parts of the integrand can be expanded for

small u, giving;

$$M_2 \approx \frac{A^2 g^2}{64\pi\mu^2}\int_0^\infty u^2 \exp(-\frac{g x_{12}}{2}u^2)du \quad (27)$$

$$\approx \frac{A^2 g^2}{64\sqrt{2\pi}\mu^2}\left(\frac{1}{g x_{21}}\right)^{\frac{3}{2}} \quad (28)$$

which gives for the two point correlation function at long distances;

$$C_{21} \approx \frac{A^2 g^{\frac{1}{2}}}{64\sqrt{2\pi}}\left[\int_0^{+\infty}\frac{d\mu}{\mu}\mathrm{e}^{-\alpha\mu}\right]\left(\frac{1}{x_{21}}\right)^{\frac{3}{2}} \quad (29)$$

A.2 Normalisation

To set the normalisation let us consider

$$C_1 = \langle|\psi_0(0)|^2\rangle \quad (30)$$

$$= \int d\mu \mathrm{e}^{-\alpha\mu} M_1 \quad (31)$$

where

$$M_1 = \int_{-\infty}^{+\infty} dV \langle 0|\mathrm{e}^{-2V}|0\rangle$$

$$= A^2\int_{-\infty}^{+\infty} dV\left[K_0\left(\sqrt{\frac{2\mu}{g}}\mathrm{e}^{-V}\right)\right]^2 \mathrm{e}^{-2V} \quad (32)$$

Again making the substitution $x = (\sqrt{2\mu/g})\mathrm{e}^{-V}$ we find that

$$\langle|\psi_0(0)|^2\rangle = \frac{A^2 g}{4}\left[\int_0^{+\infty}\frac{d\mu}{\mu}\mathrm{e}^{-\alpha\mu}\right] \quad (33)$$

A.3 Three Point Correlator

$$C_{321} = \langle|\psi_0(x_3)|^2|\psi_0(x_2)|^2|\psi_0(x_1)|^2\rangle \quad (34)$$

$$C_{321} = \int_0^{+\infty} d\mu \frac{\mathrm{e}^{-\alpha\mu}\mu^2}{2} M_3 \quad (35)$$

Inserting the resolution of unity as before;

$$M_3 = \int_0^{+\infty}\int_0^{+\infty} dE_1 dE_2 (I_1 I_2 I_3) \quad (36)$$

$$I_1 = \int_{-\infty}^{+\infty} dV_1 \langle 0|\mathrm{e}^{-2V_1(0)}|u_1\rangle \mathrm{e}^{-E_1 x_1} \quad (37)$$

$$I_2 = \int_{-\infty}^{+\infty} dV_2 \langle u_1|\mathrm{e}^{-2V_2(0)}|u_2\rangle \mathrm{e}^{(E_1-E_2)x_2} \quad (38)$$

$$I_3 = \int_{-\infty}^{+\infty} dV_3 \langle u_2|\mathrm{e}^{-2V_3(0)}|0\rangle \mathrm{e}^{E_2 x_3} \quad (39)$$

where $E_i = (g/2)u_i^2$, $i = 1, 2$. The integrals I_1 and I_3 are the same as eq. (23)whereas I_2 is a little different- introducing again the variable $x = (\sqrt{2\mu/g})\mathrm{e}^{-V}$;

$$I_2 = \frac{1}{4\pi\mu}\mathrm{e}^{(E_1-E_2)x_2}(\sinh \pi u_1 \sinh \pi u_2)^{\frac{1}{2}} \int_0^{+\infty} x dx K_{iu_1}(x) K_{iu_2}(x) \quad (40)$$

$$= \frac{1\pi}{32\mu}\mathrm{e}^{(E_1-E_2)x_2}(\sinh \pi u_1 \sinh \pi u_2)^{\frac{1}{2}} \frac{u_1^2 - u_2^2}{\cosh u_1 - \cosh u_2} \quad (41)$$

Choosing without loss of generality $x_{21} = x_2 - x_1 > 0$ and $x_{32} = x_3 - x_2 > 0$ we can use the same argument as before, that for large separations the exponentials of energy will decay very rapidly, and so the other parts of the integrand (36) can be expanded for small u_1, u_2. Then we find;

$$M_3 \approx \frac{A^2 g^3}{1024\pi\mu^3}\int_0^{+\infty} u_1^2 du_1 \exp(-\frac{g x_{21} u_1^2}{2}) \int_0^{+\infty} u_2^2 du_2 \exp(-\frac{g x_{32} u_2^2}{2}) \quad (42)$$

And we obtain for the 3 point correlation function at long distances;

$$C_{321} = \frac{A^2}{4096}\left[\int_0^{+\infty} \frac{d\mu}{\mu}\mathrm{e}^{-\alpha\mu}\right]\left(\frac{1}{x_{21}}\right)^{\frac{3}{2}}\left(\frac{1}{x_{32}}\right)^{\frac{3}{2}} \quad (43)$$

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